SciDAC
Scientific Discovery through Advanced Computing

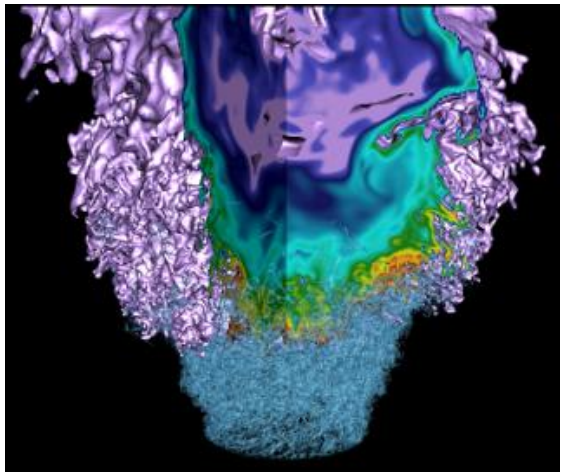
# FASTMath SciDAC Institute Overview

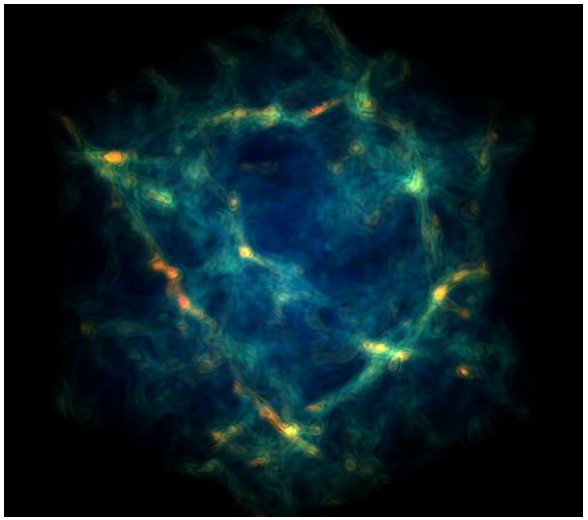
**Ann Almgren, LBNL**

Argonne NATIONAL LABORATORY
BERKELEY LAB
Sandia National Laboratories
Berkeley
COLUMBIA UNIVERSITY
Rensselaer
SMU
THE UNIVERSITY OF BRITISH COLUMBIA

# FASTMath Objectives

***The FASTMath SciDAC Institute will develop and deploy scalable mathematical algorithms and software tools for reliable simulation of complex physical phenomena and will collaborate with DOE domain scientists to ensure the usefulness and applicability of FASTMath technologies***



# The FASTMath team includes experts from four national laboratories and six universities

**Lawrence Berkeley National Laboratory**

Ann Almgren
John Bell
Phil Colella
Dan Graves
Sherry Li
Terry Ligocki
Mike Lijewski
Peter McCorquodale
Esmond Ng
Brian Van Straalen
Chao Yang

**Sandia National Laboratories**

Karen Devine
Jonathan Hu
Vitus Leung
Andrew Salinger

**Lawrence Livermore National Laboratory**

Lori Diachin
Milo Dorr
Rob Falgout
Jeff Hittinger
Mark Miller
Carol Woodward
Ulrike Yang

**Berkeley University**

Jim Demmel

**University of British Columbia**

Carl Ollivier-Gooch

**Columbia University**

Mark Adams

**Argonne National Laboratory**

Mihai Anitescu
Lois Curfman McInnes
Todd Munson
Barry Smith
Tim Tautges

**Rensselear Polytechnic Institute**

Mark Shephard
Onkar Sahni

**Southern Methodist University**

Dan Reynolds

**Colorado University at Boulder**

Ken Jansen

# FASTMath encompasses three broad topical areas

## Tools for problem discretization

- Structured grid technologies
- Unstructured grid technologies
- Adaptive mesh refinement
- Complex geometry
- High-order discretizations
- Particle methods
- Time integration

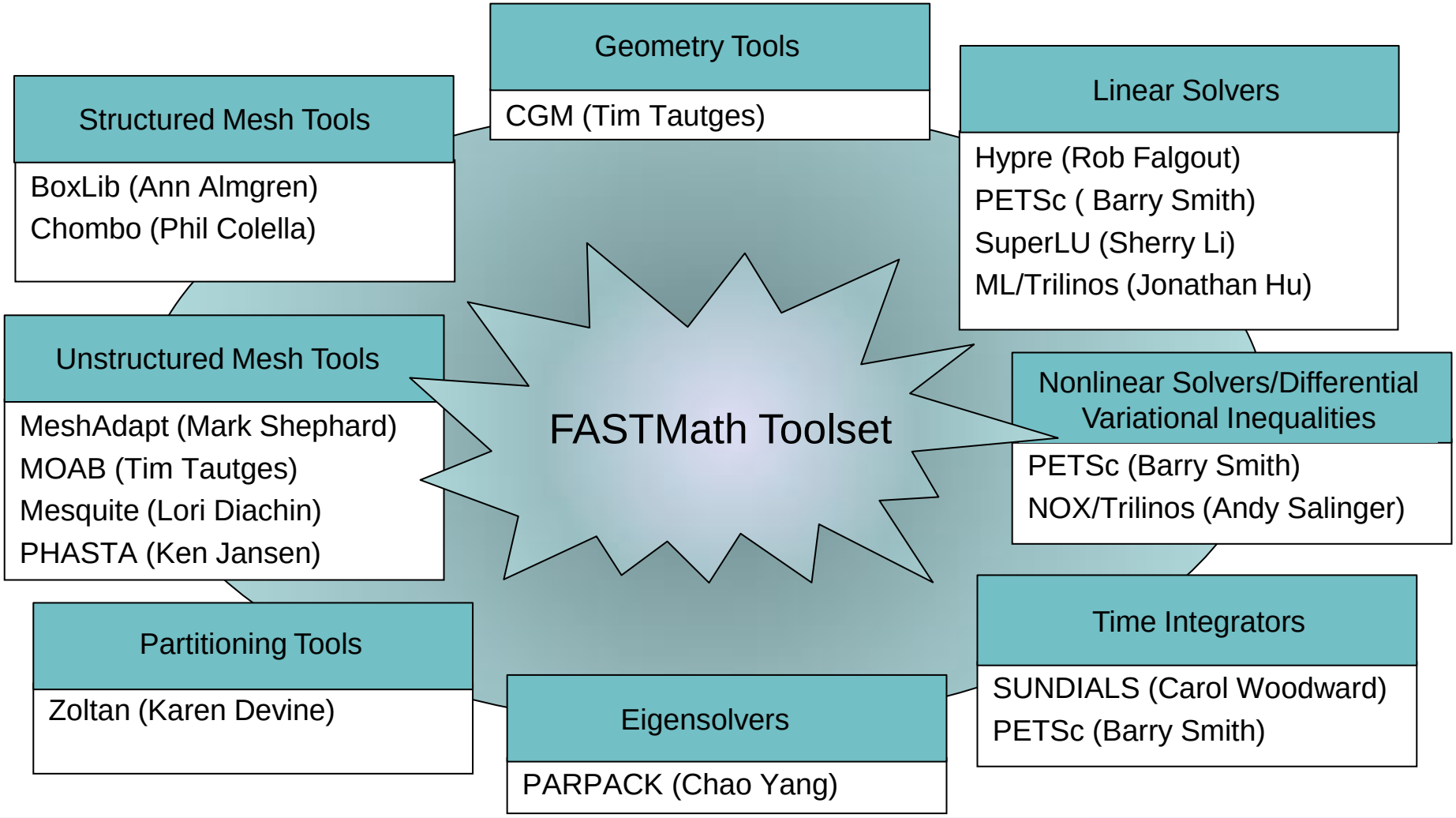
## Solution of algebraic systems

- Iterative solution of linear systems
- Direct solution of linear systems
- Nonlinear systems
- Eigensystems
- Differential Variational Inequalities

## High-level integrated capabilities

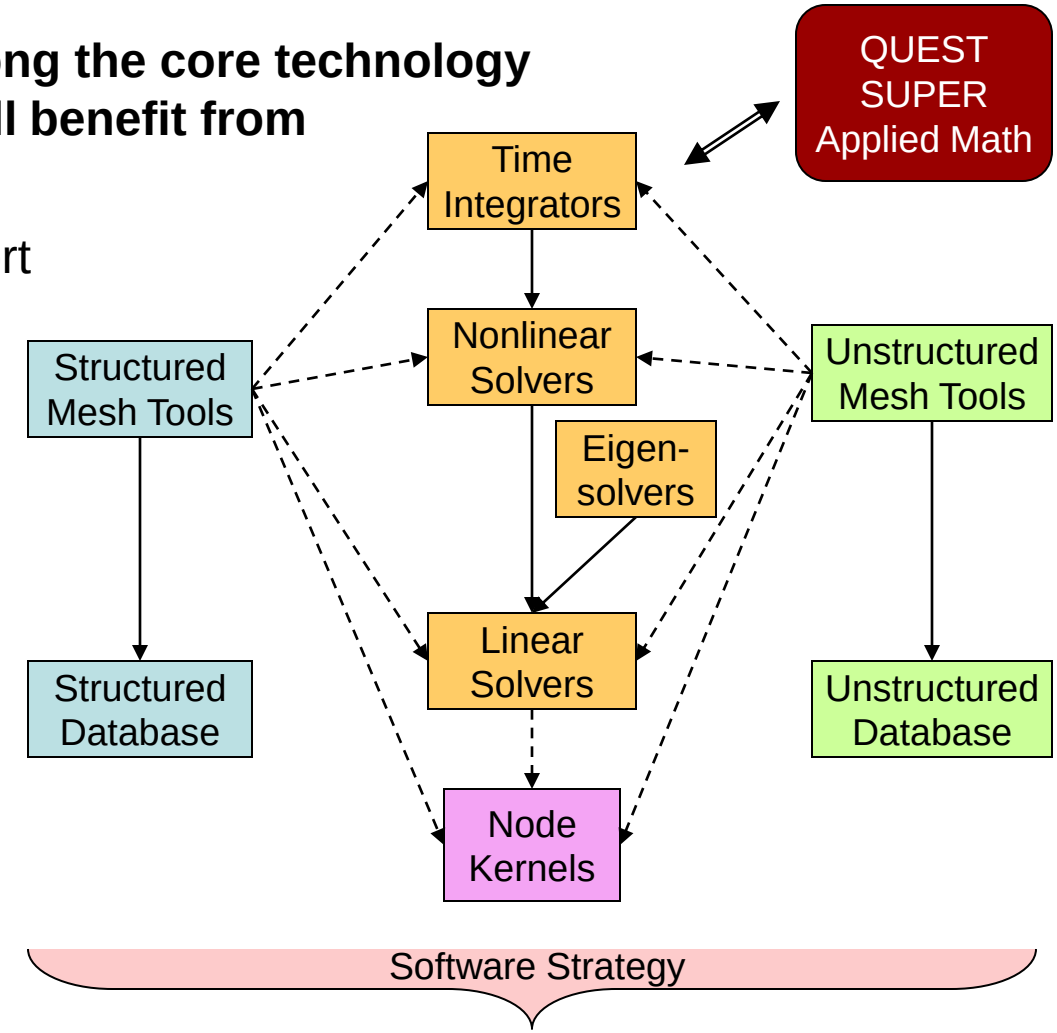
- Adaptivity through the software stack
- Management of field data
- Coupling different physical domains

# FASTMath brings a spectrum of software tools in these areas to the SciDAC Program



# FASTMath provides a unique opportunity to develop integrated capabilities

- **As we provide integration among the core technology areas, science applications will benefit from**
  - Expanded capabilities
  - Decreased development effort
- **Development efforts for expanded capability integration**:
  - Adaptivity through the software stack
  - Field data and manipulation
  - Coupling strategies for multi-physics applications
  - Architecture-aware compute node kernels
  - Unified software strategy



# All FASTMath technologies will focus on performance engineering for multi-/many-core architectures

- **MPI Parallelism**
  - Ensure all FASTMath tools operate efficiently at 10^5 to 10^6 cores
  - Architecture-aware and multi-objective partitioners for load balancing
  - Communication avoiding/hiding and latency tolerant algorithms
  - Synchronization reducing algorithms by focusing on neighborhoods, use of one-sided messages, remote memory access
- **Node-level parallelism**
  - Use of threading techniques
  - Multi-core kernels and data ordering
  - Exploit compilers, code transformation tools, programming models and run-time systems as they become available
- **Data locality**
  - Hierarchical partitioning methods and local data ordering methods
  - Shared efficient data layouts in software packages to prevent re-organization in integrated services
  - Code transformation systems, domain specific language extensions to gain performance while maintaining reusability
- **Coordinated parallelism between different levels (MPI, node, instruction)**

# Relevance to this SciDAC Project?

- **Nyx – based on BoxLib, a FASTMath-supported software framework**
  - FASTMath has paid for enhancements of subcycling and particle-mesh algorithms
  - Possible improvements in linear solvers (hypre, PETSc)?

- **Time-integration schemes?**
  - Cosmological reionization examples using IMEX schemes as part of SUNDIALS project
  - Possible improvements to handling of cosmologically relevant source terms?

- **Parallel Performance on new machines?**

- **fastmath-scidac.org**